

Report on CTTC-2022

Chemistry Division in association with the Society for Materials Chemistry (SMC) has successfully organised the DAE-BRNS symposium on the 'Current Trends in Theoretical Chemistry (CTTC-2022)' during 22-24 September 2022 at DAE convention centre, Anushaktinagar. Dr. A. K. Tyagi, Director Chemistry Group and Dr. T. Bandyopadhyay, Head, Theoretical Chemistry Section acted as the Chairman, CTTC-2022 and Chairman, Local Organising Committee respectively. Primary objective of the symposium has been to provide a vibrant platform for academic interactions and brainstorming discussions on the current trends and future directions in the field of theoretical and computational chemistry. The symposium covered a wide variety of topics that include theoretical formalisms and simulation strategies, electronic structure and spectroscopic properties of molecules, clusters and materials, chemical dynamics, reactivity and catalysis, computational biology, designing new molecules and materials for energy storage and nuclear waste management, machine learning and data mining, etc. The symposium got overwhelming response within a short span of time which clearly indicated the immense research interests in this branch of science in India and abroad. More importantly, participants are from a large number of institutes covering the length and breadth of the country with some of the most eminent researchers in the field of theoretical chemistry in India and overseas.

The symposium has been launched at 9:30 hrs on 22nd September with the inaugural function followed by an inspiring keynote address by Prof. R. B. Grover, Emeritus Professor, Homi Bhabha National Institute, Mumbai. Two Plenary Lectures have been delivered by Prof. Aurora Clark, University of Utah, USA on " Solution Chemistry in the Nuclear Fuel Cycle – Challenges and Progress in Modeling, Simulation and Data Science" and Prof. Sir Richard Catlow, University College London, UK on " Structure, Dynamics and Reactivity in Catalytic and Energy Systems". During the three days symposium, 2 Plenary Lectures, 19 Perspective talks, 12 short talks, 16 Lightning Talks and 3 technical talks were delivered by the most eminent researchers in the field that include 7 DAE faculty members. It is noteworthy to mention that great importance has been given to the young researchers by arranging large number of short and Lightning talks. All the lectures were followed by intense discussions and interaction among the participants. We received nearly 144 contributory papers for poster presentation which were loaded in the symposium

website so that all the participants can visit the posters during all the three days. Two dedicated poster sessions were also arranged for display and presenting the printed posters and selected ten posters were awarded with best poster awards. Abstracts of all the invited talks and contributory papers were published as CTTC-2022 conference proceedings. The symposium has been concluded with the concluding session on the final day where many participants applauded the efforts in organising the symposium and providing the platform for in-person interactions after the pandemic. We are confident that the symposium has provided a fertile platform for intense discussions on the recent advancements in the field of theoretical and computational chemistry, generate new ideas and concepts and enhance the knowledge of the young researchers and could lead for interdisciplinary collaborations among the leading research groups in the country. This is also expected to provide an opportunity to bring in new interdisciplinary collaborations among the theoreticians in the country.



